

Topology dependent quantities at the Anderson transition

Keith Slevin

*Dept. of Physics, Graduate School of Science, Osaka University,
1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan*

Tomi Ohtsuki

Department of Physics, Sophia University, Kioi-cho 7-1, Chiyoda-ku, Tokyo 102-8554, Japan

Tohru Kawarabayashi

Department of Physics, Toho University, Miyama 2-2-1, Funabashi 274-8510, Japan

The boundary condition dependence of the critical behavior for the three dimensional Anderson transition is investigated. A strong dependence of the scaling function and the critical conductance distribution on the boundary conditions is found, while the critical disorder and critical exponent are found to be independent of the boundary conditions.

The Anderson transition is a continuous quantum phase transition which separates metallic and insulating phases of the non-interacting electron gas [1,2]. It is expected that the critical behavior should depend only on the basic symmetry of the Hamiltonian under the operation of time reversal [3,4]. Recently this was clearly confirmed by numerical simulation [5].

At the transition the correlation length diverges and quantities such as level statistics [6,7] and the conductance distribution [5,8–10] become size independent and universal. The discovery that the critical level spacing distribution [11,12], and indications that the critical conductance distribution [13,14] also, depend on the boundary conditions was unexpected.

In this letter, we analyze both the corrections to scaling induced by different boundary conditions and the effect of the different boundary conditions on the critical disorder, critical exponent and critical conductance distribution. None of the boundary conditions we consider break time reversal symmetry, so no change in the critical behavior can be predicted on the general grounds of a transition between universality classes.

We report the results of two different simulations. In the first the scaling behavior of the localization length of electrons on long quasi-1D bars is examined. In the second the conductance distributions for ensembles of cubes of disordered material in a two probe measuring geometry are determined. Both simulations were repeated for three different boundary conditions; pbc) periodic boundary conditions in both transverse directions, mbc) periodic boundary conditions in one direction and fixed boundary conditions in the other and fbc) fixed boundary conditions in both transverse directions. These boundary conditions can be thought of as corresponding to different topologies; fbc corresponds to the topology of a wire, while mbc corresponds to that of a hollow cylinder.

We find that the location of the mobility edge separating

the localized and diffusive phases is unaffected by the choice of boundary condition. This is also true for the critical exponent. However, the scaling function of the localization length and the critical conductance distribution are found to depend strongly on the choice of boundary condition and hence on the topology of the sample.

For the numerical simulations we have used the Anderson model

$$H = V \sum_{\langle i,j \rangle} C_i^\dagger C_j + \sum_i W_i C_i^\dagger C_i, \quad (1)$$

where $C_i^\dagger (C_i)$ denotes the creation (annihilation) operator of an electron at the site i of a 3D cubic lattice. Energies W_i denote the random potential distributed independently and uniformly in the range $[-W/2, W/2]$. The hopping is restricted to nearest neighbors and its amplitude is assumed to be the energy unit, $V = 1$.

We consider first a quasi-1D system, i.e., a long bar, with cross section $L \times L$. The standard transfer matrix technique allows us to calculate the localization length of electrons $\lambda(E_F, W, L)$ on the bar within a desired accuracy [15,16]. The dependence of the quantity

$$\Lambda = \frac{\lambda(E_F, W, L)}{L} \quad (2)$$

on the width of the bar is then analyzed using the finite size scaling method. In this simulation we set the Fermi energy at the band center $E_F = 0$ and vary the strength of the random potential W and the cross section size L .

The data obtained are shown in Fig.1. In the absence of any corrections to scaling, plotting Λ vs W should show the critical disorder W_c as the common crossing point of the data. However, as seen in Fig.1, the curves for different sizes do not cross at a common point. For pbc a previous analysis [17] has suggested that main reason for this is the existence of a correction due to an irrelevant scaling variable. For mbc and fbc surface and edge contributions might also be important. Such corrections are irrelevant. For example, for a surface effect we expect the corrections vanish as L^{-1} .

To take account of corrections to scaling we use the method described in [17]. The data are fitted to the scaling form

$$\Lambda = F(\psi L^{1/\nu}, \phi L^y) \quad (3)$$

where ν is the critical exponent describing the divergence of the localization length, ϕ is the leading irrelevant variable and

y its irrelevant exponent. The best fit is found by minimizing the χ^2 statistic in the usual way.

When fitting the data, Eq.(3) is expanded in a Taylor series to first order in the irrelevant variable.

$$\Lambda = F_0(\psi L^{1/\nu}) + \phi L^y F_1(\psi L^{1/\nu}) \quad (4)$$

Both F_0 and F_1 are expanded to third order in their arguments. The relevant and irrelevant scaling variables are expanded in power series of the dimensionless disorder $w = (W_c - W)/W_c$ as follows

$$\psi = \psi_1 w \quad , \quad \phi = \phi_0 \quad (5)$$

For pbc the expansion of the relevant field in (5) was continued to quadratic order as this gave a better quality of fit. Also, for fbc, data for $L = 4$ had to be omitted in order to obtain an acceptable fit.

The numerical data and the associated fits are shown in Figs. 1,2 and 3. The estimates for the critical parameters are listed in Table I and further details of the fits in Table II. It can be seen from Fig. 1 that the main effect of imposing a fixed boundary condition at a given disorder is a decrease of the localization length λ . Also the deviations from scaling behavior are much larger than those for periodic boundary conditions. For fbc the corrections are around 15% for the smallest system size, while they are only around 2% for pbc. The estimate of the irrelevant exponent for pbc is consistent with that in [17]. The estimates for mbc and pbc are both much larger and close to $y = -1$ suggesting that the dominant correction is a surface effect.

In Fig. 2 we see that taking account of corrections to scaling by plotting $\Lambda_{\text{corrected}} = \Lambda - \phi L^y F_1(\psi L^{1/\nu})$ as the ordinate restores a common crossing point to the data for different system sizes for each boundary condition. Further the critical disorder seems to be the same for all three boundary conditions. This is reinforced by looking at Table I where 95% confidence intervals are also given. Thus the location of the mobility edge does not seem to be affected by the choice of boundary conditions. The same is true for the critical exponent.

However, the scaling function, and in particular $\Lambda_c = F_0(0)$, do depend strongly on the boundary conditions. The estimates of Λ_c given in Table I are widely separated with no overlap of the confidence intervals. The change in the estimated Λ_c is roughly 25%, while the analysis suggests that Λ_c has been estimated to within an accuracy of about 5% for fbc and to less than 1% for pbc. (Note that the apparent differences in the scaling function in the localized regime in Fig. 3 are not important; these are an artifact of the scaling procedure in which the absolute value of the correlation and localization lengths are not determined.)

Next we look at the critical conductance distribution $p_c(g)$. Since the correlation length diverges at the critical point, the critical conductance distribution of a phase coherent conductor should be scale invariant [8]. This was confirmed in numerical simulations [5,9] and it was also confirmed that $p_c(g)$ depends on the universality class [5]. The conductance of a classical conductor depends on the aspect ratio (i.e. the ratio of the cross section to the length) but not on the shape of its cross section or on its topology (i.e. whether it is a bar

or a cylinder.) Thus, a dependence of the critical conductance distribution of a quantum conductor on its aspect ratio is also expected. Whether or not the the critical conductance distribution should depend on the conductor's cross sectional shape and its topology (boundary conditions) is less clear.

We simulated the conductance distribution for an ensemble of $L \times L \times L$ cubic samples in a two probe measuring geometry using a Green's function iteration technique [18]. The conductance in units of e^2/h is

$$g = 2\text{tr}(tt^\dagger) \quad (6)$$

where t is the transmission matrix found in the Green's function iteration and the factor of two takes account of spin degeneracy.

We first simulated an ensembles of 1,000,000 systems for each boundary condition. The resulting distributions are shown in Fig. 4. The choice of boundary condition affects $p_c(g)$ especially for small g . There is a tendency towards more insulating behavior for fbc.

It is expected on general grounds that $p_c(g)$ will be size independent for "large enough" system sizes. This leaves open the possibility that the dependence of $p_c(g)$ on the boundary conditions in Fig. 4 may simply be an indication that the system sizes employed in our work are not "large enough". We therefore decided to examine the size dependence of $p_c(g)$. The dependence of $\langle g \rangle$ on the size L for $L = 4$ to $L = 20$ for each boundary condition is shown in Fig. 5. Ensembles of 100,000 systems were generated for each system size with the exceptions of $L = 16$ and $L = 20$ where the ensemble sizes were reduced to 25,000 and 10,000 respectively.

To estimate the asymptotic value of $\langle g \rangle$ in the limit $L \rightarrow \infty$ we have assumed that the size dependence is due to an irrelevant scaling variable and fitted the data to

$$\langle g(L) \rangle = \langle g(\infty) \rangle + aL^y. \quad (7)$$

The details of the fits are given in Table III. From the results it seems clear that the boundary condition dependence will not disappear as $L \rightarrow \infty$. The asymptotic value of the mean conductance is reduced by about 40% while the analysis suggests that it has been estimated to within a few percent. The numerical data are consistent with a size independent and universal $p_c(g)$ but also one that depends on the boundary conditions even in the limit $L \rightarrow \infty$.

The size dependence of the critical conductance fluctuations were analyzed in a similar way and the results are also given in Table III. (For fbc no size dependence of the variance was detected within the accuracy of the simulation so the value given is simply a weighted average over different system sizes.) The values given can be compared with the value of $\text{var}(g)=1.18$ (with g in units of e^2/h) for universal conductance fluctuations in the metallic regime [19]. Though the absolute magnitude of the fluctuations is smaller than in the metallic regime, the conductance fluctuations are in fact of the same order of magnitude as $\langle g \rangle$ at the transition.

The estimates of the irrelevant exponent in Table III again suggest the presence of surface effects. However, for the conductance calculation it seems to be pbc which presents a surface effect rather than fbc. For the latter boundary condition a surface correction does not seem to be present and we find a

value of the irrelevant exponent which is consistent with that for the scaling behavior of the localization length with pbc given in Table I.

In conclusion we have found that the some aspects of the critical behavior at the Anderson transition, the location of the mobility edge and the critical exponent, are independent of the boundary conditions. Other aspects, the scaling function and the critical conductance distribution, seem to depend strongly on the boundary conditions. The invariance of the critical disorder is reasonable since localized states should be unaffected by boundary conditions. However, this argument does not hold in the critical regime and, as we have shown, important aspects of the critical behavior do depend on the topology. The exception is the critical exponent provided, as here, that the boundary conditions do not break time reversal symmetry.

Finally, we recall that a similar dependence of the scaling functions on boundary conditions has also been found in classical percolation [20,21]. This suggests that the quantum nature of the Anderson transition might not be crucial for the existence of this sort of effect.

The authors would like to thank K.Fukushima, S.Todo, Y.Okabe and N.Hatano for useful discussions.

75, 193 (1995).

[21] J. Cardy, J. Math. Gen. **17** L385 and L967 (1984).

	ν	W_c	Λ_c	y
pbc	1.56(55,58)	16.54(53,55)	0.576(.574,.577)	-2.8(3.2,2.4)
mbc	1.60(56,64)	16.47(42,52)	0.502(.494,.509)	-1.3(1.5,1.2)
fbc	1.54(41,61)	16.49(39,64)	0.426(.403,.442)	-1.2(1.4,1.0)

TABLE I. The best fit estimates of the critical exponent, the critical disorder, Λ_c and the irrelevant exponent together with their 95% confidence intervals.

	N_d	N_p	χ^2	Q
pbc	336	12	335	0.3
mbc	238	11	233	0.4
fbc	204	11	212	0.2

TABLE II. The boundary condition, the number of data N_d , the number of parameters N_p , the value of χ^2 for the best fit and goodness of fit Q . The system sizes used were $L = 4, 5, 6, 8, 10, 12, 14$ with the exception of fbc where the data for $L = 4$ were omitted and pbc where data for $L = 16$ are also included. The accuracy of the numerical data was either 0.1% or 0.05%. The range of disorder used was $W = 15$ to $W = 18$.

	$\langle g(\infty) \rangle$	Q	y'	$\text{var}(g(\infty))$
pbc	$0.89 \pm .02$	0.2	$-0.9 \pm .1$	$0.472 \pm .01$
mbc	$0.71 \pm .01$	0.6	$-1.1 \pm .1$	$0.408 \pm .003$
fbc	$0.560 \pm .002$	0.9	$-2.3 \pm .7$	$0.349 \pm .001$

TABLE III. The estimated value of $\langle g \rangle$ in the thermodynamic limit $L \rightarrow \infty$ together with standard errors, the goodness of fit Q and an estimate of the irrelevant exponent. An estimate of $\text{var}(g)$ in the limit $L \rightarrow \infty$ together with standard errors is given in the last column.

- [1] P. Anderson, Phys. Rev. **109**, 1492 (1958).
- [2] P. A. Lee and T. V. Ramakrishnan, Revs. Mod. Phys. **57**, 287 (1985).
- [3] F. Wegner, Z. Phys. **B25**, 327 (1976).
- [4] E. Abrahams *et al.*, Phys. Rev. Lett. **42**, 673 (1979).
- [5] K. Slevin and T. Ohtsuki, Phys. Rev. Lett. **78**, 4083 (1997).
- [6] B.I. Shklovskii, B. Shapiro, B.R. Sears, P. Lambrianides and H.B. Shore, Phys. Rev. **B47**, 11487 (1993).
- [7] I. Kh. Zharakeshev and B. Kramer, Phys. Rev. Lett. **79**, 717 (1997).
- [8] B. Shapiro, Phys. Rev. Lett. **65**, 1510 (1990).
- [9] P. Markos and B. Kramer, Phil. Mag. **B68**, 357 (1993).
- [10] P. Markos, Phys. Rev. Lett. **83**, 588 (1999).
- [11] D. Braun, G. Montambaux and M. Pascaud, Phys. Rev. Lett. **81**, 1062 (1998).
- [12] V.E. Kravtsov and V. I. Yudson, Phys. Rev. Lett. **82**, 157 (1999).
- [13] C.M. Soukoulis, X. Wang, Q. Li and M.M. Sigalas, Phys. Rev. Lett. **82**, 668 (1999).
- [14] K. Slevin and T. Ohtsuki, Phys. Rev. Lett. **82**, 669 (1999).
- [15] A. MacKinnon and B. Kramer, Z. Phys. **B53**, 1 (1983).
- [16] B. Kramer and A. MacKinnon, Rep. Prog. Phys. **56**, 1469 (1993).
- [17] K. Slevin and T. Ohtsuki, Phys. Rev. Lett. **82**, 382 (1999).
- [18] T. Ando, Phys. Rev. **B44**, 8017 (1991).
- [19] P. A. Lee, A. D. Stone and H. Fukuyama, Phys. Rev. **B35**, 1039 (1987).
- [20] C.-K. Hu, C.-Y. Lin, and J.-A. Chen, Phys. Rev. Lett.

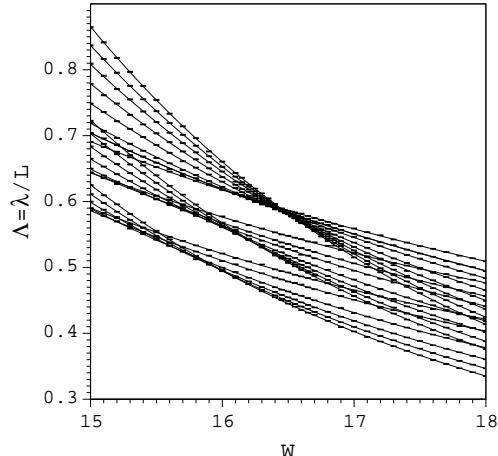


FIG. 1. Λ vs. W . for periodic (upper curves), mixed (middle curves) and fixed (lower curves) boundary conditions.

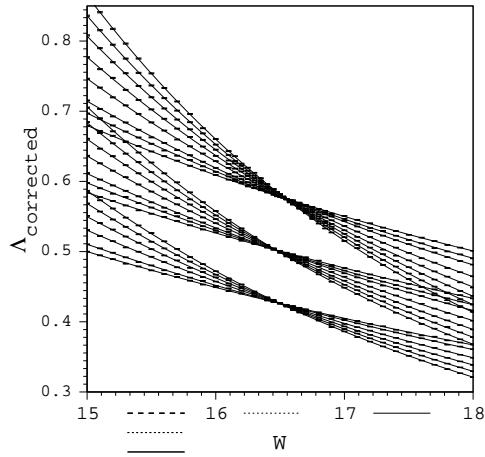


FIG. 2. Λ vs. W after the surface corrections are removed.

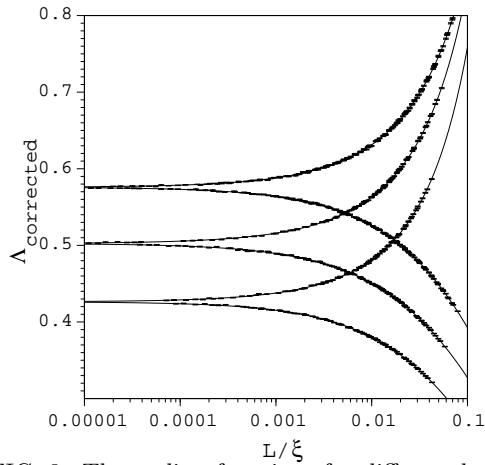


FIG. 3. The scaling functions for different boundary conditions.

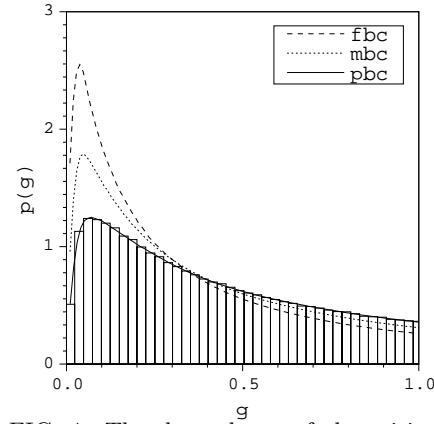


FIG. 4. The dependence of the critical conductance distribution on the choice of boundary conditions. Here the Fermi energy $E_F = 0$, the system size $L = 10$ and the disorder $W = 16.54$ independent of the choice of boundary conditions.

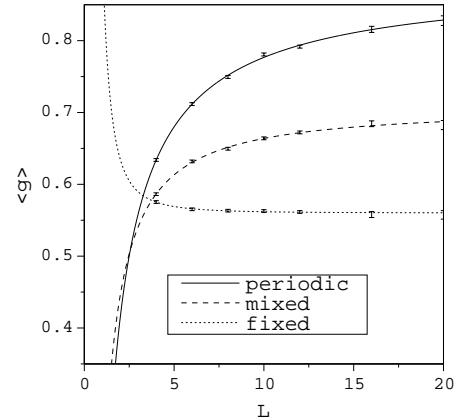


FIG. 5. The size dependence of $\langle g \rangle$ for different boundary conditions. Here the Fermi energy $E_F = 0.5$ for which we estimated $W_c = 16.53$ independent of the choice of boundary conditions.